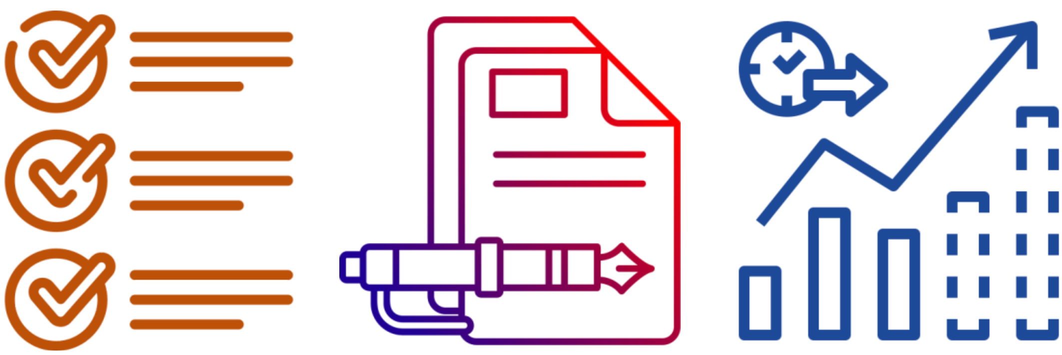
CHAPTER 7

Summary, Conclusion and Future Aspects



7.1. Summary and Conclusions

Liquid crystals are integral to modern life, prominently used in a variety of applications such as displays for televisions, smartphones, computer monitors and medical devices due to their unique ability to modulate light efficiently. Advancements in liquid crystal technology have led to significant improvements in display quality, including higher resolution, faster response times and enhanced colour reproduction. Beyond displays, liquid crystals are now utilized in advanced optical devices, sensors and tuneable lenses, showcasing their versatility. Despite these advancements, there is a pressing need for the development of new liquid crystalline materials. This need arises from the desire to further enhance performance characteristics, improve energy efficiency and address environmental concerns associated with the production and disposal of liquid crystal devices. Developing liquid crystalline materials is crucial to mitigate continued innovation and application of this versatile technology in a wide range of fields. A novel library of liquid crystal molecules is needed to explore new structural varieties and properties, enabling the discovery of materials with superior characteristics.

The primary objective of this research was to synthesize a diverse range of novel homologous liquid crystal compounds, encompassing various structural motifs mainly cholesterol-based Schiff's bases and heterocyclic derivatives. These compounds were then subjected to comprehensive characterization using analytical techniques including elemental analysis, spectroscopy (FT-IR, ^{1}H-NMR, ^{13}C-NMR), microscopy and thermal analysis, to elucidate their molecular structure, physical properties and mesomorphic behaviour. The synthesized compounds' photophysical properties, including photoluminescence and photoisomerization, were investigated to assess their potential applications in optoelectronic devices and materials. Furthermore, the antioxidant properties of the synthesized liquid crystal compounds were evaluated using DPPH assays, aiming to explore their potential as antioxidants in various applications. Biological activities against bacteria and fungi were also assessed to investigate their potential as antimicrobial agents. Density Functional Theory (DFT) calculations were performed to provide theoretical insights into the electronic structure, optical properties and molecular behaviour of the synthesized liquid crystal compounds, aiding in the interpretation of experimental results and guiding further research directions.

The outcomes of this research suggest that the synthesized liquid crystal materials exhibit promising properties for diverse applications in fields such as optoelectronics, materials science and biomedical engineering. The findings contribute to the understanding of structure-property relationships in liquid crystal materials and provide a basis for the development of novel compounds with enhanced properties and applications.

In conclusion, this thesis thoroughly investigates a diverse array of novel liquid crystal compounds containing cholesterol and various heterocyclic moieties with different functional groups. Each chapter provides unique perspectives and creative methodologies about different liquid crystalline compounds that enrich the comprehensive investigation.

Chapter 1 serves as a foundational introduction to the multifaceted realm of liquid crystals. It offers a comprehensive historical overview, tracing the evolution of liquid crystal research from its inception to contemporary advancements. Additionally, the chapter explores the classification of liquid crystals, elucidating the diverse structural arrangements and mesophase transitions observed in these materials. Furthermore, it explores into the complex relationship between molecular structure and the resulting mesomorphic properties, highlighting the importance of molecular design in tailoring liquid crystal behaviour. Finally, Chapter 1 examines the broad spectrum of applications where liquid crystals play a pivotal role, spanning fields such as display technology, telecommunications, sensors and biomedical engineering. Through a thorough exploration of these topics, Chapter 1 sets the stage for the subsequent chapters, laying the groundwork for a deeper understanding of the fascinating world of liquid crystals.

In **Chapter 2**, we have synthesized twenty-six new mesogenic Schiff's base derivatives (1a-m and 1' a-m) by condensing 4-n-alkoxy aniline with 4-formyl phenyl cholesteryl carbonate and 4-formyl 3-methoxy phenyl cholesteryl carbonate, all exhibiting mesomorphic properties. The methyl to n-hexyl derivatives display an enantiotropic chiral nematic mesophase, while the n-pentyl and n-hexyl derivatives also show an additional TGB_A-SmA monotropic mesophase. The n-heptyl to n-decyl derivatives exhibit enantiotropic TGB_A-SmA and N* phase transitions, while the n-dodecyl to n-octadecyl derivatives show enantiotropic SmA and SmC* mesophases. Increasing terminal chain length results in stronger emission and higher fluorescence quantum yield, with all compounds showing moderate to good antioxidant activity. The effect of lateral methoxy substitution is also examined, revealing a reduction in thermal stability and mesophase stability. DFT calculations provide insights into theoretical chemical reactivity, highlighting areas of low and high electron density. The investigation of their application aspects holds significant potential.

The study in **Chapter 3**, outlines a systematic approach to synthesizing homologous cholesterol-based azo-biphenyl liquid crystalline compounds with diverse alkoxy side chains, all displaying mesogenic properties. The methyl to n-hexyl derivatives exhibit enantiotropic chiral nematic mesophases, while the n-heptyl to n-decyl compounds transition from SmA to isotropic phases with a TGBA phase in between. Higher homologues, from n-dodecyl to n-octadecyl, demonstrate enantiotropic SmA mesophases. Transition temperature plots show a sharp decrease in N*/SmA to isotropic transition temperatures and an increase in SmA to N* transition with increasing terminal chain length. These compounds display good thermal stability (297 to 338 °C) and moderate antioxidant activity. Additionally, they exhibit photoisomerization behaviour in dilute solutions. Theoretical chemical reactivity studies, utilizing Density Functional Theory calculations, focus on Frontier Molecular Orbitals and Molecular Electrostatic Potential mapping to identify energy gaps and electron density regions. Their photoswitching properties make them promising candidates for electronic and optical device applications, with potential uses in light-responsive displays, data storage devices and smart windows.

In **Chapter 4**, we have successfully designed and synthesized thirteen new homologues by condensing 4-formyl phenyl cholesteryl carbonate with 5-(4'-n-alkoxyphenyl)-2-amino-1,3,4-thiadiazole, exhibiting multiple mesophases including chiral nematic (N*), twist grain boundary-A (TGB_A), smectic A (SmA) and chiral smectic C (SmC*) phases. The plot of transition temperature versus number of carbon atoms in the alkoxy chain reveals a rising trend for the smectic A to chiral nematic curve with increasing terminal chain length, while the smectic C* to smectic A shows a falling tendency. Some mesogen exhibit good to moderate radical scavenging activity. Additionally, all compounds are UV-active and demonstrate photoluminescence in the blue emission region. With longer terminal chain lengths, there is a noticeable increase in emission intensity and fluorescence quantum yield, corroborated by DFT studies indicating lower energy gaps in Frontier MOs, indicative of enhanced fluorescence emission. DFT calculations further elucidate theoretical chemical reactivity, including analysis of Frontier MOs and MEP mapping, providing insights into regions of low and high electron density.

In **Chapter 5**, thirteen novel liquid crystalline compounds are synthesized through the condensation of 5-(4'-n-alkoxy phenyl)-2-amino-1,3,4-oxadiazole with 4-n-methoxybenzoyloxy benzaldehydes. All compounds 8a-m exhibit mesomorphism. The methyl to n-pentyl derivatives demonstrate an enantiotropic nematic phase, while the n-hexyl to n-decyl derivatives show an enantiotropic SmA-N-Isotropic transition. Additionally, the n-dodecyl to n-octadecyl derivatives display an enantiotropic SmA mesophase. The n-hexadecyl and n-octadecyl homologues exhibit a monotropic SmC mesophase transition during cooling. In the plot correlating transition temperature with the number of carbon atoms in the alkoxy chain, the Smectic A to nematic curve peaks, while the Smectic A to Smectic C transition (during cooling) declines. All compounds exhibit UV activity and photoluminescence in the blue emission region. Increased terminal chain length results in stronger emission and higher fluorescence quantum yield. Additionally, all compounds demonstrate moderate to good antioxidant activity. Theoretical chemical reactivity studies using DFT calculations focus on Frontier MOs and MEP mapping to determine energy gaps and electron density regions.

In **Chapter 6**, four new Schiff's bases are synthesized by condensing 2-amino-1,3-thiazole with four different substituted formyl phenyl cholesteryl carbonates and investigated for their anti-microbial, anti-oxidant, mesogenic, optical and thermal properties. While the compounds do not exhibit better radical scavenging activity compared to standards, all derivatives demonstrate significant to moderate levels of antibacterial and antifungal activities. Only one derivative, 7a (without substituted core), shows a mesogenic property, exhibiting a chiral nematic mesophase (N*). All derivatives are UV-active and exhibit photoluminescence in the blue emission spectrum. Thermal analysis results indicate that slight changes in molecular structures alter the overall thermal stability of the resultant molecules. The derivatives show moderate drug-likeness and bioactivity scores. Theoretical chemical reactivity studies, considering Frontier MOs and MEP mapping, predict high and low electron density areas, highlighting potential interacting sites for biological activity and confirming the liquid crystalline property.

7.2. Future Aspects

1. **Novel Compounds to Be Explored Further:** Future attempts can be made to explore and synthesize additional liquid crystal compounds containing different structural motifs and functional groups. Future research may involve using more classes of compounds that are synthesized by enlarging the library in terms of the molecular architectures with a possible finding of better compound properties and mesophase behaviours respectively.

2. **Application-Based Research:** Future studies will need to investigate practical applications for these synthesized liquid crystal compounds in optoelectronics, materials science and biomedical engineering among other fields. This can include studying them for use in specific applications like drug release systems, photonic devices, sensors or as part of displays.

3. **More Optimization for Molecular Design:** Moreover, further research work should also focus on optimizing the mesomorphic behaviour, thermal stability and optical properties through fine-tuning of molecular design of LCs which may involve systematic modification of molecular structures and functional groups till desired effects are attained.

4. **Theoretical and Computational Studies:** Future investigations could delve deeper into theoretical and computational studies using techniques like DFT calculations. These studies can provide valuable insights into the electronic structure, optical properties, and chemical reactivity of liquid crystal compounds, aiding in the design and prediction of novel materials.

5. **Biomedical Applications:** Given the promising antibacterial and antifungal activities demonstrated by some synthesized compounds, future research could explore their potential applications in biomedical fields such as antimicrobial coatings, wound dressings or drug delivery systems. Further studies could also investigate their biocompatibility and cytotoxicity profiles.

6. **Environmental Impact Assessment:** As new liquid crystal compounds are developed and synthesized, it is important to consider their potential environmental impact. Future research could include extensive environmental assessments evaluating factors such as biodegradability, eco-toxicity as well as long-term effects on ecosystems.

By addressing these future aspects, researchers can continue to advance the field of liquid crystals thereby unlocking new opportunities for innovation and tackling critical issues confronting materials science and technology.